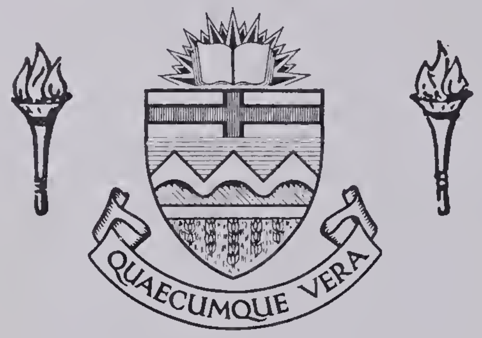
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RAPID NUMERICAL SOLUTION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

by

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled RAPID NUMERICAL SOLUTION TO THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION, submitted by William Isaac Newman, in partial fulfillment of the requirements for the degree of Master of Science.

ABSTRACT

The objective of this thesis is to show that the exact solution to the one-dimensional Schrödinger equation may be obtained everywhere in terms of "smoothly-varying" functions at a speed controlled by Hamilton's equations if the numerical techniques employed embody a <u>methodological</u> compatibility with the <u>conceptual</u> link between wave and particle mechanics.

The thesis begins by examining the historical development of numerical techniques for solving the one-dimensional Schrödinger equation in the context of preserving a smooth numerical link between classical and quantum mechanical solutions of equations of motion. The problem of calculating the wave function in the allowed and forbidden regions is reformulated as that of obtaining a correction to a semiclassical asymptotic form; at the same time, this introduces the need for solving a Riccati equation for a function $\phi(x)$ and an associated "phase correction function" $f(x)$. The relation between these functions is discussed stressing the properties of bounding, the behaviour at the turning point and the particular solution to the equation for $\phi(x)$ which satisfies the requirement that the wave function become the complex exponential of a modified form of Hamilton characteristic function. A new method

for obtaining the solution to a particular class of Riccati equations (including the *desired* solution to $\phi(x)$) is presented in the context of a "linearized iterative sequence." Its implementation in two rapid numerical algorithms is discussed and tested. Finally, results are given which conclusively show that the wave function may be precisely obtained with the speed of solving the Hamilton-Jacobi equations of motion in the region where JWKB approximants are valid.

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CHAPTER I

INTRODUCTION

An important mathematical problem in quantum mechanics is that of solving the one-dimensional Schrödinger equation

$$\frac{d^2y(x)}{dx^2} + k^2(x)\ y(x) = 0 \tag{1.1}$$

where

$$k^2(x) = \frac{2m}{\hbar^2}\ [E - V(x)]\ . \tag{1.2}$$

This equation, a form of Sturm-Liouville problem, was first investigated in a purely mathematical context by Carlini (1817), Liouville (1837), and Green (1837). The advent of quantum mechanics revived interest in the problem and the search for useful approximate solutions led to the rediscovery or development of the JWKB approximation (after Jeffreys(1) (1923)), Wentzel, Kramers, and Brillouin (1926)),

$$y(x) = (|k(x)|)^{-\frac{1}{2}} \exp[\pm i \int^{x} k(x')dx' + \varepsilon(x)]\ . \tag{1.3}$$

This approximation is valid (that is, the correction function $\varepsilon(x)$ is negligibly small) only in an asymptotic domain where $k(x)$ is non-zero and $[k'(x)/k(x)]$

is sufficiently small. Zeros of k(x) are called "turning points," a name which alludes to the properties of the corresponding classical motion. The solution to Schrödinger's equation in the form (1.3) is characterized by a "phase" describing the wave properties of the probability amplitude for a quantum mechanical particle and an amplitude describing an essentially classical variation of probability density with the reciprocal of the particle momentum. The JWKB approximation is of interest not only <u>physically</u>, because of the interpretation which can be given to the amplitude and the leading term of the phase, but <u>mathematically</u>, since these quantities, unlike the wave function y(x), do not oscillate but vary smoothly in a fashion controlled by the classical momentum. When sufficiently accurate, the JWKB asymptotic form is thus computationally far superior to direct integration of the Schrodinger equation (1.1), particularly when the de Broglie wavelength $2\pi/k(x)$ is small.

These properties of the JWKB approximation have stimulated other workers to investigate its properties further with the intent of extending its range of validity and accuracy and, possibly, its physical interpretation. While certain aspects of the mathematical problem of such asymptotic series solutions to

these equations go back as far as the work of Green (1837), discussions having a direct bearing on the physical interpretation of solutions to Schrödinger's equation are more recent. In this connection, we shall mention the efforts of two workers as a résumé of relevant work.

Langer$^{(2)}$ considered the Schrodinger wave function to have the form

$$y(x) = \exp[\lambda \int^{x} \sigma(x',\lambda)\ dx'] \tag{1.4}$$

from which one obtains a Riccati equation for σ (where λ is large)

$$\frac{\sigma'(x)}{\lambda} + \sigma^2(x) + p^2(x) = 0 \tag{1.5}$$

where

$$p(x) = [k(x)/\lambda] \quad . \tag{1.6}$$

If $\sigma(x,\lambda)$ is represented as a series expansion in λ^{-1}, that is

$$\sigma(x,\lambda) = \sum_{j=0}^{\infty} [\frac{\sigma_j(x)}{\lambda^j}] \quad , \tag{1.7}$$

the differential equation becomes

$$(\sigma_o^2(x) + p^2(x)) + \sum_{j=1}^{\infty} \lambda^{-j} [\sigma'_{j-1}(x) + \sum_{\ell=0}^{j} \sigma_\ell(x)\, \sigma_{j-\ell}(x)] = 0 . \tag{1.8}$$

By choosing the coefficients $\sigma_j(x)$ so that individual terms vanish, that is,

$$\sigma_o(x) = \pm ip(x),\ \sigma_j(x) = [-1/2\ \sigma_o(x)]\{\sigma'_{j-1}(x) + \sum_{\ell=1}^{j-1} \sigma_\ell(x)\, \sigma_{j-\ell}(x)\} , \tag{1.9}$$

the equation is formally solved. Langer saw that a solution of this type is apparently asymptotic and may not be extended across the turning points. Since a zero of $k^2(x)$ is a singular point of the asymptotic equation exactly solved by (1.3) (with $\varepsilon(x) = 0$), a "Stokes' phenomenon" occurs, that is, an analytic solution $y(x)$ to equation (1.1) which is asymptotically well represented by a particular linear combination of the asymptotic forms (1.3) on one side of a zero of $k^2(x)$ will <u>not</u> be asymptotically well represented by the <u>same</u> linear combination of the corresponding analytic continuations of the forms (1.3) on the other side of the zero; a "Stokes' jump" occurs in the linear

combination coefficients. Langer showed that a "connection formula" fixing the Stokes' jumps can be obtained using the asymptotic expansions of solutions to Airy's equation (assuming that $k^2(x)$ is approximately linear in x in the neighbourhood of its zeros).

There are several known alternative expansions of the JWKB forms to that of Langer. They all agree up to second order, which is the form (1.3) with $\varepsilon = 0$. This fact, plus the difficulty of computing higher terms, their lack of obvious physical interpretation, and the relatively poor subsequent convergence of all such expansions has led to the widespread adoption of (1.3) as the standard JWKB form.

Kemble$^{(3)}$, following Zwaan, considered the wave function to be a linear combination of such second-order JWKB forms, that is

$$y(x) = \alpha_+\hat{W}_+(x) + \alpha_-\hat{W}_-(x) \tag{1.10}$$

in the classically allowed region (where k(x) is real) and

$$y(x) = \beta_+\hat{W}_+(x) + \beta_-\hat{W}_-(x) \tag{1.11}$$

in the classically forbidden region (where k(x) is imaginary) with $\hat{W}_\pm(x)$ defined by

$$\hat{W}_{\pm}(x) = (|k(x)|)^{-\frac{1}{2}} \exp[\pm i \int^{x} k(x')dx'] \ . \qquad (1.12)$$

Owing to the Stokes phenomenon, α_+, α_- are not equal to β_+, β_-; by developing exact equations for the way in which these asymptotically constant coefficients change along a path in the complex plane circumnavigating the turning point on the real axis, Kemble succeeded in obtaining a rigorous derivation of the connection formulae without appealing to Airy's equations as a model. Kemble's approach is of interest to our work because of its emphasis on the connection to exact solutions to (1.1) of the coefficients $\alpha_{\pm}(x)$.

The work of Langer and Kemble is a pinnacle of achievement in the formulation of the JWKB method although the literature on the subject before and after their work is enormous. A much more recent book by Fröman and Fröman$^{(4)}$ (1965) compiles and summarizes the known literature and the reader is referred to this work for a more complete bibliography than can be given here.

One further analytic outgrowth of the JWKB method is of direct interest to us. Regular solutions of Schrödinger's equation associated with scattering by a central potential are asymptotically characterized by a JWKB solution (that is, a linear combination of forms (1.3)) with a characteristic amplitude and

"phase-shift," the latter constant fixing the ratio of the linear combination coefficients. It then seems natural to characterize the exact regular solution everywhere in the classically allowed region by a JWKB form connected by *variable* phase and amplitude functions which would assume the correct asymptotic values at infinity. Much of the work on these techniques is due to or has been summarized in the book by Calogero(5). However, all of Calogero's methods have a serious defect: the differential equation for the variable phase shift and all subsequent modifications of it possess a "step-like" behaviour in the phase function (associated with trigonometric cycles in the wave function) so that, although this correction to the JWKB form is small, its rapid variation at such "steps" makes the technique of relatively little numerical advantage.

The advent of the high-speed digital computer has fostered the growth of numerical techniques in solving the one-dimensional Schrödinger equation. Essentially, these are truncated Taylor series expansions which are used recursively to calculate the wave function and its derivatives at a set of points which are separated by some small but finite length or step-size. Such techniques have two serious limications.

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One is that truncated Taylor expansions contain an error term which is bounded by the stepsize. Therefore, to make the calculation reliable, it is necessary to select the stepsize to be significantly smaller than the local wavelength $2\pi/k(x)$ of the Schrödinger equation. The second limitation is due to the finite precision of computers. Since two linearly independent solutions to Schrödinger's equation exist, imprecise calculations will introduce a component of the irregular solution which will eventually diverge. Thus, in making the stepsize sufficiently small to ensure the accuracy of the truncated Tayler series, the number of calculations will decrease the precision of the calculations thereby promoting the growth of the undesirable and non-physical solution.

In an effort to minimize the growth of the irregular solution, Gordon(6) has proposed that the potential energy be regarded as a collection of piecewise continuous line segments. Then, in any one of these segments, Schrödinger's equation takes the form

$$\frac{d^2y(z)}{dz^2} - z\,y(z) = 0 \qquad (1.13)$$

which has Airy function solutions, namely

$$\begin{aligned} A_i(-z) &= \frac{1}{3}\sqrt{z}\,\{J_{1/3}(\tfrac{2}{3}z^{3/2}) + J_{-1/3}(\tfrac{2}{3}z^{3/2})\} \\ B_i(-z) &= \sqrt{\frac{z}{3}}\,\{J_{-1/3}(\tfrac{2}{3}z^{3/2}) - J_{1/3}(\tfrac{2}{3}z^{3/2})\}\ . \end{aligned} \qquad (1.14)$$

By suitably matching these wave functions at the boundaries of the line segments, the wave function for the entire range may be constructed. Gordon's method is superior to a direct numerical integration in terms of the accuracy and the speed with which the calculations may be performed. Unfortunately, both techniques are numerical methods only and offer no physical insight into the problem.

From the preceding survey of numerical techniques for solving the one-dimensional Schrödinger equation, one obtains a feeling of methodological discontinuity; in the presently existing repertory, there seems to be no technique which takes advantage of any conceptual link between quantum mechanics and classical mechanics. In classical mechanics, one integrates Hamilton's equations or, equivalently, the Hamilton-Jacobi equations, and the stepsize for numerical integration is limited only by the rate at which the potential function changes with respect to the local energy; in the exact integration of the Schrödinger equation, on the other hand, the de Broglie wavelength $2\pi/k(x)$ determines the stepsize in place of the natural stepsize for Hamilton's equations, except when the latter is smaller (as in the case of low energy). In the high energy limit, the JWKB approximation recovers an estimate of

the solution which can be made at the speed of Hamilton's equations, but there is no simple technique which permits a smooth extension by numerical methods to the exact solution without introducing the discontinuity of method and corresponding difficulty represented, for example, by the much smaller stepsize of the direct integration of Schrödinger's equation. The motivation for this work lay in the persistent feeling that this discontinuity of numerical method and accompanying numerical difficulty could in fact be eliminated, and, as we shall see, this feeling is correct.

A clue to the origins of the discontinuity of method is provided if one examines the nature of the conceptual link between quantum and classical mechanics, and this link, of course, involves the JWKB approximation. Quantum mechanics replaces the classical concept of a point particle in motion with that of a moving wave packet. The size of the packet, a measure of the uncertainty in the particle's position, is proportional to Planck's constant. Thus, in the limit that $\hbar$ goes to zero, quantum mechanics and classical mechanics should provide the same description of matter. It is well-known(7) that, in this limit, the Schrödinger equation becomes equivalent to the Hamilton-Jacobi

equations of motion provided that the wave function has the form

$$y(x) = \exp\{i\,S(x)/\hbar\} \qquad (1.15)$$

where S(x) is Hamilton's characteristic function, namely

$$S(x) = \int^{x} \sqrt{2m[E - V(x')]}\ dx' \ . \qquad (1.16)$$

It is important to note that this solution is identical to Langer's when λ becomes infinite. (Langer's definition of $\sigma_o(x)$ includes an indeterminacy in its sign as a result of taking the square root of a quantity. In the classical picture, this corresponds to a particle whose momentum has a well-defined magnitude but whose direction of motion is purely left going or purely right going.) Moreover, if one assumes λ to be $1/\hbar$, then Langer's formal solution to the Riccati equation may be interpreted as the classical solution followed by a perturbation series in $\hbar$. Furthermore, the term p(x) is identically the classical momentum. Therefore, $[-i\sigma(x)]$ is the "quantum mechanical momentum" and possesses the classical momentum as its leading term followed by a perturbation series in $\hbar$. Indeed, this is consistent with the momentum-operator equation

$$-i\hbar \frac{dy(x)}{dx} = [-i\sigma(x)]\ y(x) \quad . \qquad (1.17)$$

If, therefore, one wishes to preserve a smooth <u>numerical</u> link between classical and quantum mechanical solutions of equations of motion, the preceding discussion strongly suggests that one pay special attention not to the general solution of Schrödinger's equation but to those two particular solutions which, in the classical limit, correspond to a momentum eigenfunction, that is the solutions of Schrödinger's equations which also asymptotically obey (1.17). We shall see that the greater numerical difficulty of previous techniques for exact solution of Schrödinger's equation is entirely the result of attempting a direct calculation of a general solution of the form

$$y(x) = A(x) \begin{matrix}\sin\\ \cos\end{matrix}\left\{\int^{x} p(x')dx' + \delta(x)\right\} \quad . \qquad (1.18)$$

Such a wave function poses conceptual difficulties when one tries to make the transition to classical mechanics, because it describes the superposition of <u>two</u> equiprobable states of a quasi-classical particle (left and right going waves); conversely, the apparently discontinuous increase in the difficulty of obtaining an exact numerical solution on going from classical to

quantum mechanics might be due entirely to using (1.18) rather than the "complex exponential" solutions as the particular exact solutions to be generated. In other words, the intimate asymptotic connection between complex exponential solutions and Hamilton's characteristic function suggests that they can be *exactly* calculated with the ease and speed of solving the Hamilton-Jacobi equations.

CHAPTER II

REFORMULATION OF THE PROBLEM AS A CORRECTION TO AN ASYMPTOTIC FORM

A. Classically Allowed Region

Define functions $\alpha_{\pm}(x)$ so that the solution to the one-dimensional Schrödinger equation has the form

$$y(x) = \alpha_{+}(x)W_{+}(x) + \alpha_{-}(x)W_{-}(x)$$

$$y'(x) = \alpha_{+}(x)W_{+}'(x) + \alpha_{-}(x)W_{-}'(x) \qquad (2.1)$$

where

$$W_{\pm}(x) = \exp\{\pm i \int_{x_o}^{x} k(x')dx'\} \quad . \qquad (2.2)$$

This solution corresponds with a linear combination of two asymptotic exponential solutions to Schrödinger's equation. The coefficients are allowed to vary continuously so that the wave equation will be satisfied exactly. Our selection of $W_{\pm}(x)$ to be non-singular at the turning point (unlike Kemble's choice) suggests that, by suitably obtaining the coefficients $\alpha_{\pm}(x)$, the wave function will be regular everywhere.

By simultaneously solving equations (2.1), the coefficients are observed to be

$$\alpha_{\pm}(x) = \pm \left\{\frac{y(x)W_{\mp}'(x) - y'(x)W_{\mp}(x)}{-2ik(x)}\right\} . \qquad (2.4)$$

This expression may be simplified by defining a new set of coefficients $\beta_{\pm}(x)$ by

$$\beta_{\pm}(x) = \alpha_{\pm}(x) \{-2ik(x)\} \qquad (2.5)$$

so that

$$\beta_{\pm}(x) = \pm \{y(x)W_{\mp}'(x) - y'(x)W_{\mp}(x)\} . \qquad (2.6)$$

Differentiating once and employing the explicit form for $W_{\pm}(x)$ and the wave equation for $y(x)$, the problem reduces to that of solving

$$\beta_{\pm}'(x) = g(x)\{\beta_{\pm}(x) + \beta_{\mp}(x)\exp[\mp \int_{x_o}^{x} h(x)dx]\} \qquad (2.7)$$

where $g(x)$ and $h(x)$ are defined by

$$g(x) = \frac{k'(x)}{2k(x)}$$
$$(2.8)$$
$$h(x) = 2ik(x) \quad .$$

This equation may be further simplified by eliminating the diagonal coupling in the equation. Defining new coefficients $\gamma_{\pm}(x)$ by

$$\beta_{\pm}(x) = \gamma_{\pm}(x)\ \exp\{\int_{x_o}^{x} g(x')dx'\}\ , \qquad (2.9)$$

one finds that

$$\gamma_{\pm}'(x) = \gamma_{\mp}(x)\ g(x)\ \exp\{\mp \int_{x_o}^{x} h(x')dx'\}\ . \qquad (2.10)$$

Coupled first-order differential equations of this form have been investigated in the theory of inelastic atomic collisions. In particular, Lebeda and Thorson(8) found that undesirable and spurious double-frequency oscillations in numerical solutions to such equations were generated by inappropriate usage of initial conditions and that these could be suppressed by introducing a suitable asymptotic solution form. They defined coefficients $b_+(x)$ and $b_-(x)$ by

$$\begin{aligned} b_+(x) &= \gamma_+(x) \\ b_-(x) &= \gamma_-(x)\ \exp\{-\int_{x_o}^{x} h(x')dx'\} \end{aligned} \qquad (2.11)$$

from which one obtains the following pair of coupled equations:

$$\begin{aligned} b_-'(x) + h(x)b_-(x) &= b_+(x)g(x) \\ b_+'(x) &= b_-(x)g(x)\ . \end{aligned} \qquad (2.12)$$

Lebeda and Thorson were led to introduce such an asymmetric bias into the symmetric equations (2.10) by the physical initial conditions for inelastic scattering which provided that asymptotically $\gamma_{+}(x)$, say, has the value 1 while $\gamma_{-}(x)$ goes to zero (in that problem, the coefficients represent amplitudes for initial and final states, respectively, before collision). Why should solutions possessing an asymptotic asymmetrical bias of this sort be of interest in our present problem? A posteriori we may appeal to the intuition of Chapter I which emphasizes that it is the "pure complex exponential" solutions which bear a direct interpretive connection to the motion of a classical particle.

Following Lebeda and Thorson, therefore, suppose that we consider a particular solution of (2.1) for which $\alpha_{-}(x)$ is very much smaller, at least asymptotically, than $\alpha_{+}(x)$; then $\gamma_{-}(x)$ will be much smaller than $\gamma_{+}(x)$. Since, then, $\gamma_{-}(x)$ will be largely "driven" by $\gamma_{+}(x)$ via the coupled equations (2.10), it is reasonable and consistent to think that the asymmetrically biased quantities $b_{\pm}(x)$ will both be slowly varying. The coupled equations for $b_{\pm}(x)$ may be converted to a single Riccati equation

$$\phi(x) = \frac{g(x)}{h(x)} \{1 - \phi^2(x)\} - \frac{\phi'(x)}{h(x)} \qquad (2.13)$$

and a quadrature

$$b_+(x) = b_+(x_o)\exp\{\int_{x_o}^{x} \phi(x')g(x')dx'\} , \qquad (2.14)$$

where

$$\phi(x)b_+(x) = b_-(x) \quad . \qquad (2.15)$$

Now, any attempt to numerically integrate equation (2.13) would only re-introduce the oscillations we wish to avoid. However, it is immediately of interest to observe that far from a turning point, an approximate solution of (2.13) is

$$\phi(x) \approx \frac{g(x)}{h(x)} \quad ; \qquad (2.16)$$

indeed, if $[g(x)/h(x)]$ is sufficiently small, it is evident that such a solution for ϕ would justify the rationale in selecting the transformations for $b_\pm(x)$, namely that $b_-(x)$ is small and $b_\pm(x)$ is slowly varying. But $[g(x)/h(x)]$ small is just the condition for asymptotic validity of the JWKB approximation.

It is now desirable to construct the wave function in terms of $\phi(x)$. It is useful to observe that

$$\exp\{\int_{x_o}^{x} g(x')dx'\} = \sqrt{\frac{k(x)}{k(x_o)}} \quad . \qquad (2.17)$$

Combining these with the transformations made earlier, the $\alpha_\pm(x)$ coefficients become

$$\alpha_+(x) = \alpha_+(x_o)\sqrt{\frac{k(x)}{k(x_o)}}\,\exp\{\int_{x_o}^{x}\phi(x')g(x')dx'\}$$

$$\alpha_-(x) = \phi(x)\exp\{\int_{x_o}^{x} h(x')dx'\}\alpha_+(x) \quad . \qquad (2.18)$$

Is this result consistent with the assumptions made in constructing the various transformations, namely that the magnitude of $\alpha_-(x)$ is much smaller than the magnitude of $\alpha_+(x)$? Since $h(x)$ is pure imaginary, the exponential term does not alter the magnitude of $\alpha_-(x)$. Thus, only the magnitude of $\phi(x)$ is significant. By equation (2.15), $\phi(x)$ can be approximated by $k'(x)/4ik^2(x)$ which is small in the region where the JWKB approximation is valid. Therefore, equations (2.18) are indeed consistent with the assumptions that have been employed.

With this understanding, the wave function and its derivative (neglecting proportionality constants common to both) may be written

$$y(x) = [1+\phi(x)][k(x)]^{-\frac{1}{2}}\exp\{i\int_{x_o}^{x}[k(x)-\frac{ik'(x)}{2k(x)}\phi(x)]dx\}$$

$$y'(x) = i[1-\phi(x)][k(x)]^{\frac{1}{2}}\exp\{i\int_{x_o}^{x}[k(x)-\frac{ik'(x)}{2k(x)}\phi(x)]dx\}. \qquad (2.19)$$

Note that when $\phi(x)$ is zero, these expressions are identically those of the "pure exponential" second order JWKB approximant. Thus, even the crudest estimate of $\phi(x)$ can give very accurate wave functions. This form preserves the wave character of the solution (as a pure right going wave) and describes the classical variation of probability density with the reciprocal of the particle's momentum. However, the nature of the solution at the turning point is unknown and the general form of the solution is not conveniently that of a complex exponential. We shall discover later how these difficulties may be circumvented.

In the preceding discussion, it was assumed that $\alpha_+(x)$ dominated $\alpha_-(x)$, that is to say, the wave was right going. Consider, to the contrary, that $\alpha_-(x)$ dominates $\alpha_+(x)$; i.e. that the wave is left going. Then, select coefficients $b_+(x)$ and $b_-(x)$ by

$$\begin{aligned} b_+(x) &= \gamma_+(x) \exp\left\{ \int_{x_o}^{x} h(x)dx \right\} \\ b_-(x) &= \gamma_-(x) \end{aligned} \tag{2.20}$$

with the corresponding pair of coupled equations

$$\begin{aligned} b_+'(x) - h(x)b_+(x) &= b_-(x)g(x) \\ b_-'(x) &= b_+(x)g(x) \quad . \end{aligned} \tag{2.21}$$

This may be converted to a single Riccati equation, namely

$$\phi(x) = -\frac{g(x)}{h(x)}\{1-\phi^2(x)\} + \frac{\phi'(x)}{h(x)} \tag{2.22}$$

where

$$\phi(x) = \frac{b_+(x)}{b_-(x)} \quad . \tag{2.23}$$

An approximate solution to this equation, valid far from the turning point is

$$\phi(x) = -\frac{g(x)}{h(x)} \quad . \tag{2.24}$$

It is important to note that equation (2.22) is the complex conjugate of equation (2.13); therefore, one need only calculate $\phi(x)$ for one of these equations since the solution to the other will be its complex conjugate. For this reason, $\phi(x)$ will be used to denote the solution to (2.13) whereas $\phi^*(x)$ will denote the solution to (2.24). In identical fashion, one obtains the wave function and its derivative for a left going wave to be

$$\begin{aligned} y(x) &= [1+\phi^*(x)][k(x)]^{-\frac{1}{2}}\exp\{-i\int_{x_o}^{x}[k(x)+\frac{ik'(x)}{2k(x)}\phi^*(x)]dx\} \\ y'(x) &= [1-\phi^*(x)][k(x)]^{\frac{1}{2}}\exp\{-i\int_{x_o}^{x}[k(x)+\frac{ik'(x)}{2k(x)}\phi^*(x)]dx\} . \end{aligned} \tag{2.25}$$

This solution to the wave function may immediately be recognized as the complex conjugate to (2.19). Thus, any general solution to Schrödinger's equation may be expressed as a linear combination of (2.19) and its complex conjugate; it is significant that this includes all <u>real</u> solutions. This technique must now be applied to the task of calculating the wave function in the forbidden region.

B. Classically Forbidden Region

The first portion of this chapter formulated a technique for obtaining the solution to the one-dimensional Schrödinger equation in the allowed region as a correction to an asymptotic form. To extend this technique into the forbidden region, consider the solution to the wave equation to have the form

$$\begin{aligned} y(x) &= \alpha_+(x)W_+(x) + \alpha_-(x)W_-(x) \\ y'(x) &= \alpha_+(x)W_+'(x) + \alpha_-(x)W_-'(x) \end{aligned} \qquad (2.26)$$

where

$$W_\pm(x) = \exp\{\pm\int_{x_0}^{x} k(x)dx\} \quad . \qquad (2.27)$$

The detailed calculations are identical in form to those employed earlier. For the sake of brevity, one need only recognize that the mapping

$$k(x) \longrightarrow -ik(x) \tag{2.28}$$

will transform the equations which describe the allowed region into those which describe the forbidden region. Thus, g(x) and h(x) become

$$\begin{aligned} g(x) &= \frac{k'(x)}{2k(x)} \\ h(x) &= 2k(x) \quad . \end{aligned} \tag{2.29}$$

For the case that $\alpha_+(x)$ dominates $\alpha_-(x)$, the solution to the wave equation may be written

$$\begin{aligned} y(x) &= [1+\phi(x)][k(x)]^{-\frac{1}{2}}\exp\{\int_{x_o}^{x}[k(x)+\frac{k'(x)}{2k(x)}\phi(x)]dx\} \\ y'(x) &= [1-\phi(x)][k(x)]^{\frac{1}{2}}\exp\{\int_{x_o}^{x}[k(x)+\frac{k'(x)}{2k(x)}\phi(x)]dx\} \end{aligned} \tag{2.30}$$

where $\phi(x)$ satisfies

$$\phi(x) = \frac{g(x)}{h(x)}\{1-\phi^2(x)\} - \frac{\phi'(x)}{h(x)} \quad . \tag{2.31}$$

Note that, in the region far from the turning point, $\phi(x)$ is approximately

$$\phi(x) \approx \frac{g(x)}{h(x)} \quad . \tag{2.32}$$

For the case that $\alpha_-(x)$ dominates $\alpha_+(x)$, the solution to the wave equation may be written

$$y(x) = [1+\phi(x)][k(x)]^{-\frac{1}{2}} \exp\left\{\int_{x_o}^{x} [-k(x) + \frac{k'(x)}{2k(x)}\phi(x)]dx\right\}$$

$$y'(x) = [1-\phi(x)][k(x)]^{+\frac{1}{2}} \exp\left\{\int_{x_o}^{x} [-k(x) + \frac{k'(x)}{2k(x)}\phi(x)]dx\right\} \tag{2.33}$$

where $\phi(x)$ satisfies

$$\phi(x) = -\frac{g(x)}{h(x)}\{1-\phi^2(x)\} + \frac{\phi'(x)}{h(x)} \quad . \tag{2.34}$$

Far from the turning point, $\phi(x)$ is given approximately by

$$\phi(x) \approx -\frac{g(x)}{h(x)} \quad . \tag{2.35}$$

In both of these cases, $\phi(x)$ is a real-valued function, unlike its counterpart in the allowed region which has both real and imaginary components. Thus, it is no longer possible to construct a solution to the latter equation for $\phi(x)$ as the complex conjugate of the solution to (2.31). However, this is not important since only one solution to the wave equation is required (that is, the decaying mode) in the forbidden region.

* * *

This chapter commenced by reformulating the problem of solving the one-dimensional Schrödinger equation as a correction to asymptotic solutions of exponential form. In pursuing this approach, a pair of solutions was obtained in both allowed and forbidden regions which bear a striking resemblance to pure exponential JWKB approximants, and which reduces to them in the asymptotic limit ($k'(x)/k(x)$ and its derivatives sufficiently small). Such a form preserves the concept of the phase of a wave <u>and</u> the classical variance of the probability density with reciprocal particle momentum. In the semiclassical domain, a good approximate solution for the function $\phi(x)$ will generate a solution $y(x)$ which is more accurate than the JWKB solution.

The crucial question, of course, is the nature of the particular solution $\phi(x)$ to equation (2.13) which is embodied in the solution $y(x)$ in (2.19) and whose asymptotic leading term is the small quantity given by (2.16). Is this $\phi(x)$ bounded, especially at the turning point? Is it a smooth function of x or does it exhibit oscillatory or step-like behaviour which would destroy any numerical utility of this approach? We were originally led to consider the analogy with the problem of Lebeda and Thorson because they found that an <u>iterative</u> solution of their Riccati equation analogous

to (2.13), starting with the zero-order approximation (2.16), was indeed a smooth function without the spurious oscillations they wished to eliminate. (The meaning of an "iterative solution" to a non-linear equation may be clarified by consulting a reference such as Mathews and Walker(9). It is explicitly shown there that, in the case of the JWKB problem, iteration gives rise to the first two terms of the Langer series.) It turns out that a modified form of the iterative method generates a smooth $\phi(x)$ but we defer discussion of this subject until the iterative solution of equation [(2.13), (2.19), (2.31), (2.34)] is described in Chapter IV. The boundedness of $\phi(x)$ is significant since we hope to obtain a form for the wave function which remains non-singular through the turning point region. Finally, the form of the solution (2.19) appears to abandon our original suggestion that a "physical" solution should be the pure exponential of a modified Hamilton's characteristic function, that is, a smoothly-varying function of the potential. In the next chapter, we shall resolve most of these questions.

CHAPTER III

PURE EXPONENTIAL WAVE FUNCTION

A. Derivation of Pure Exponential Form of Solution

The preceding chapter succeeded in reformulating the problem of solving the one-dimensional Schrödinger equation as a correction to an asymptotic form. As a consequence, we seemingly have abandoned the ideal of obtaining a pure exponential solution. Consider, then, the ratio of equations (2.19),

$$\frac{y'(x)}{y(x)} = ik(x) \left\{\frac{1 - \phi(x)}{1 + \phi(x)}\right\} \quad . \tag{3.1}$$

This may be regarded as a linear first order differential equation in y(x). The corresponding first integral is

$$y(x) = \exp \left\{i \int_{x_o}^{x} k(x) \left[\frac{1 - \phi(x)}{1 + \phi(x)}\right] dx\right\} \tag{3.2}$$

where $\phi(x)$ is determined by (2.13). A second solution which is valid in the allowed region is its complex conjugate

$$y^*(x) = \exp \left\{-i \int_{x_o}^{x} k(x) \left[\frac{1 - \phi^*(x)}{1 + \phi^*(x)}\right] dx\right\} \quad . \tag{3.3}$$

Similarly, the solutions which are valid in the forbidden region are

$$y(x) = \exp \{\pm \int_{x_o}^{x} k(x) \ [\frac{1 - \phi_{\pm}(x)}{1 + \phi_{\pm}(x)}] \ dx\} \qquad (3.4)$$

where $\phi_+(x)$ and $\phi_-(x)$ satisfy (2.31) and (2.34) respectively. Now that solutions to the wave equation which are simultaneously momentum eigenfunctions have been formally defined, it is necessary to investigate the properties of $\phi(x)$ and its calculation.

B. Phase Correction Function

The pure exponential character of the solution just obtained imparts much significance to a quantity we shall call $f(x)$ where

$$f(x) = \frac{1 - \phi(x)}{1 + \phi(x)} \ . \qquad (3.5)$$

The function $f(x)$ has the effect of modifying the JWKB phase; for this reason, it shall be referred to as the "phase correction function". However, unlike the phase correction function employed by some techniques, this one provides the amplitude of the wave function as well.

The function $\phi(x)$ is related to $f(x)$ by

$$\phi(x) = \frac{1 - f(x)}{1 + f(x)} \ . \qquad (3.6)$$

Equations (3.5) and (3.6) are examples of linear fractional transformations$^{(10)}$. Such a transformation maps lines into circles and circles into lines. Of particular interest is the fact that (3.5) maps the region of complex ϕ-space bounded on the outside by the unit circle into the right-half complex plane.

This symmetrization may be extended to the differential equations which define $\phi(x)$, namely

$$\begin{aligned} \phi(x) &= \frac{G(x)}{2H(x)}\{1-\phi^2(x)\} - \frac{\phi'(x)}{H(x)} \\ f(x) &= \frac{H(x)}{2G(x)}\{1-f^2(x)\} - \frac{f'(x)}{G(x)} \end{aligned} \tag{3.7}$$

where

$$G(x) = \frac{k'(x)}{k(x)} \tag{3.8}$$

and

$$H(x) = \begin{cases} 2ik(x) & \text{(allowed region)} \\ 2k(x) & \text{(forbidden region)}\ . \end{cases} \tag{3.9}$$

Therefore, we see that if a formal solution $\phi(x)$ be obtained as some functional $Q[G(x),H(x)]$, then the functional $Q[H(x),G(x)]$ is a solution for $f(x)$; however, it is <u>not</u>, in general, the <u>corresponding solution</u> defined by (3.6). Hence, such a symmetrical relation is not of direct interest.

Certain symmetry properties of sets of solutions $\phi(x)$ and their corresponding $f(x)$ are of interest. We noted earlier that the complex conjugate of any solution to equation (2.13) is a solution to equation (2.22). In addition, the reciprocal of any solution to (2.13) (or (2.31) in the forbidden region) is a solution to (2.22) (or (2.34) in the forbidden region). An equally intriguing result is that, if $\phi(x)$ is a solution to (2.31) and corresponds with some $f(x)$, then $1/\phi^*(x)$ is also a solution to (2.31) which, by inspection, corresponds with $-f^*(x)$. Extending this unusual relationship between the equations which define $\phi(x)$ for left and right going waves to the phase correction function, this corresponds with replacing $f(x)$ in, say, the left going solution

$$y(x) = \begin{cases} \exp\left\{i \int_{x_o}^{x} k(x)\, f_{left}(x)dx\right\} & \text{(allowed region)} \\ \exp\left\{\int_{x_o}^{x} k(x)\, f_{left}(x)\, dx\right\} & \text{(forbidden region)} \end{cases} \qquad (3.10)$$

with $-f(x)$ in the right going solution

$$y(x) = \begin{cases} \exp\left\{-i \int_{x_o}^{x} k(x)\, f_{right}(x)dx\right\} & \text{(allowed region)} \\ \exp\left\{- \int_{x_o}^{x} k(x)\, f_{right}(x)dx\right\} & \text{(forbidden region)} \end{cases} \qquad (3.11)$$

and, consequently, recovers an identical solution to the wave equation. Yet another way of looking at this relationship between the equations for $\phi(x)$ is that they are identical up to the selection of the branch cut in evaluating $k(x)$. Thus, if one knows the general solution to $\phi(x)$ determined by one differential equation, the general solution to the complementary differential solution is also known.

The initial condition for the equation for $\phi(x)$ in the allowed region was observed, in the preceding chapter, to be that $\phi(x)$ varies as $k'(x)/4ik^2(x)$ far from the turning point. Is this consistent with the pure exponential form of solution obtained in this chapter? Consider the integrand of (3.2)

$$\begin{aligned} k(x)f(x) &= k(x)\{\frac{1-\phi(x)}{1+\phi(x)}\} \\ &= k(x)\{1 - 2\phi(x) + O[\phi^2(x)]\} \ . \end{aligned} \tag{3.12}$$

Compare this with the first two terms of the JWKB (or Langer) series

$$k(x) + \frac{ik'(x)}{2k(x)} = k(x) \ \{1 + \frac{ik'(x)}{2k^2(x)}\} \quad . \tag{3.13}$$

By associating $-2\phi(x)$ with $+ik'(x)/2k^2(x)$, the comparison is complete. Moreover, this shows that $f(x)$ is given approximately by

$$f(x) = 1 + \frac{ik'(x)}{2k^2(x)} \qquad (3.14)$$

far from the turning point. Similar results hold in the forbidden region.

The exponential solution which has been obtained describes, in the semiclassical limit, a particle movin a particular direction. The phase correction function f(x) provides for deviation in amplitude and phase of a quantum mechanical particle from its classical counterpart: however, if the qualitative concept of a particular direction to the particle's motion (and, hence, the specific idea of a "pure complex exponential" solution) is to retain any validity, the complex function f(x) must remain in the same half of the complex plane (namely, the right half) for all points x in the classically allowed domain. From the linear fractional transformation (3.6), this in turn requires that $\phi(x)$ lie within the unit circle. In Appendix A, a proof is given that if $\phi(x_o)$ satisfies this condition at some point x_o in the classically allowed domain, then $\phi(x)$ will be so bounded for all points in the domain. Therefore, the above concepts remain valid. This illustrates a crucial difference between the problem of calculating $\phi(x)$ (or f(x)) and that of calculating phase and amplitude factors associated with other techniques: the function $\phi(x)$ is

bounded! All that is now required is a technique for calculating it in various regions.

C. Iterative Solution to the Riccati Equation for $\phi(x)$

Consider the general first order Ricatti equation

$$\psi(x) = \alpha(x) + \beta(x)\psi^2(x) + \gamma(x)\psi'(x) \ . \tag{3.15}$$

The following iterative scheme is proposed whenever $\alpha(x)$, $\beta(x)$ and $\gamma(x)$ are analytic, "small" compared with unity, and have slowly varying derivatives.

For $i = 0, 1, 2, \ldots$, a solution to (3.15) may be obtained by solving the ancillary equation

$$\psi_i(x) = \alpha_i(x) + \beta_i(x)\psi_i^2(x) + \gamma_i(x)\psi_i'(x) \tag{3.16}$$

by invoking a natural recurrence scheme

$$\psi_i(x) = \psi_{i+1}(x) + \alpha_i(x) \tag{3.17}$$

where

$$\begin{aligned} \delta_i(x) &= 1 - 2\alpha_i(x)\beta_i(x) \\ \alpha_{i+1}(x) &= \{\beta_i(x)\alpha_i^2(x) + \gamma_i(x)\alpha_i'(x)\}/\delta_i(x) \\ \beta_{i+1}(x) &= \beta_i(x)/\delta_i(x) \\ \gamma_{i+1}(x) &= \gamma_i(x)/\delta_i(x) \end{aligned} \tag{3.18}$$

given that

$$\begin{aligned} \alpha_o(x) &= \alpha(x) \\ \beta_o(x) &= \beta(x) \\ \gamma_o(x) &= \gamma(x) \quad . \end{aligned} \tag{3.19}$$

From these relations, it follows that the required solution to (3.15) is given by $\psi_o(x)$, namely

$$\psi(x) = \psi_o(x) = \sum_{i=0}^{\infty} \alpha_i(x) \quad . \tag{3.20}$$

This recursion scheme is consistent with the formulation of the equations for $\phi(x)$ and may be applied directly.

For convenience, define $U(x)$ and $P(x)$ by

$$\begin{aligned} U(x) &= k^2(x) \\ P(x) &= \frac{U'(x)}{4U(x)} \quad . \end{aligned} \tag{3.21}$$

(Note that the discussion here is valid only in the allowed region. However, by making the mapping (2.28), this analysis is equally valid in the forbidden region.) Then observe that

$$\begin{aligned} \alpha(x) &= \frac{1}{2ik(x)} P(x) \\ \beta(x) &= -\frac{1}{2ik(x)} P(x) \\ \gamma(x) &= -\frac{1}{2ik(x)} \quad . \end{aligned} \tag{3.22}$$

By the explicit use of the preceding recurrence relations, one finds

$$\alpha_o(x) = \frac{1}{2ik(x)} P(x)$$

$$\beta_o(x) = - \frac{1}{2ik(x)} P(x)$$

$$\gamma_o(x) = - \frac{1}{2ik(x)} \tag{3.23}$$

$$\alpha_o'(x) = \frac{1}{2ik(x)} \{\frac{U''(x)}{4U(x)} - 6P^2(x)\} \quad .$$

Noting that

$$P'(x) = \frac{U''(x)}{4U(x)} - 4P^2(x) \tag{3.24}$$

one finds

$$\alpha_1(x) = \{\frac{1}{4ik(x)} P(x) + \frac{U''(x)}{8U(x)} - 3P^2(x)\}/C(x)$$

$$\beta_1(x) = ik(x)P(x)/C(x)$$

$$\gamma_1(x) = ik(x)/C(x) \tag{3.25}$$

$$\alpha_1'(x) = \{- \frac{P^4(x)}{2ik(x)} + \frac{P^2(x)P'(x)}{2ik(x)} + \frac{U'''(x)}{8U(x)}$$

$$- 6P(x)P'(x) - 2\,\alpha_1(x)[U'(x)$$

$$- P(x)P'(x)]\}/C(x)$$

where C(x) is defined by

$$C(x) = 2U(x) - P^2(x) \ . \qquad (3.26)$$

Since $\alpha_2(x)$ is given by

$$\alpha_2(x) = \{\beta_1(x)\alpha_1^2(x) + \gamma_1(x)\alpha_1'(x)\}/$$

$$\{1 - 2\alpha_1(x)\beta_1(x)\} \ , \qquad (3.27)$$

$\phi(x)$ may be approximated by

$$\phi(x) \approx \alpha_o(x) + \alpha_1(x) + \alpha_2(x) \ . \qquad (3.28)$$

Such an iterative scheme for calculating $\phi(x)$ can be carried out numerically to any order by methods described in Chapter IV and, where it shows acceptable numerical convergence, leads to essentially exact results for $\phi(x)$ and the corresponding solution $y(x)$ to the Schrödinger equation. This iterative expansion for $\phi(x)$ appears to be either asymptotic or convergent and is very much more accurate than the JWKB form (1.3) over essentially the entire semiclassical domain where the latter provides a reasonable approximation; on the other hand, when the JWKB approximation deteriorates, the iterative process diverges.

What we wish to emphasize here, however, is not the detail of methods for evaluating this particular solution $\phi(x)$, but rather the fact that such a particular

solution exists and that it can be determined to extraordinary accuracy over the semiclassical domain; furthermore, as noted earlier and as desired originally, this solution is smoothly varying and does not present any oscillatory or step-like behaviour. In the cases where no domain of semiclassical behaviour exists, that is, cases for which the JWKB approximation is nowhere valid, the de Broglie wavelength is not significantly smaller than the characteristic dimensions of the potential surface and, thus, there would be no computational advantage in integrating at the speed of Hamilton's equations over direct numerical integration of the second-order Schrödinger equation.

Given that a semiclassical domain exists in which an accurate "iterative" estimate of this particular solution $\phi(x)$ of (2.13) can be made, we must then consider its analytic properties so that, if possible, we can obtain its approximate analytic or numerical continuation into the domains where the iterative scheme for calculating it fails. To this end, we now consider properties of this solution (and its corresponding phase correction function $f(x)$) in the turning point region.

D. Behaviour of the Desired $\phi(x)$ in the Turning Point Region

Since, in equations (3.7), the roles of G(x) and H(x) are interchanged when going to the equation for f(x) from that for $\phi(x)$, it is tempting to consider the use of the iterative solution scheme to obtain a particular solution for f(x) in the neighbourhood of a turning point, where $k^2(x) = 0$:

$$f(x) = \frac{ik^2(x)}{k'(x)} \{1 - f^2(x)\} - \frac{k(x)}{k'(x)} f'(x). \qquad (3.29)$$

In Appendix B, we discuss the particular solutions f(x) which can thus be obtained. However, it turns out that such a solution for f(x) does not at all correspond with the particular $\phi(x)$ which interests us. The asymptotic behaviour of the desired $\phi(x)$ in the neighbourhood of a turning point may be deduced as follows:

Recall that the equation which determined $\phi(x)$ is (after some rearrangement)

$$\phi'(x) + h(x)\phi(x) = g(x)\{1 - \phi^2(x)\}. \qquad (3.30)$$

Consider the substitution

$$\phi(x) = \text{Tanh}\ \{\frac{u(x)}{4}\} \quad . \qquad (3.31)$$

The differential equation then obtained for u(x) is

$$\frac{u'(x)}{4} \mathrm{Sech}^2 \{\frac{u(x)}{4}\} + h(x) \mathrm{Tanh} \{\frac{u(x)}{4}\}$$

$$= g(x) \mathrm{Sech}^2 \{\frac{u(x)}{4}\} \quad . \qquad (3.32)$$

In the vicinity of the turning point, h(x) vanishes and one must solve

$$u'(x) = 4g(x)$$

$$= \frac{2k'(x)}{k(x)} \quad . \qquad (3.33)$$

This is an exact differential and one finds that

$$\frac{u(x)}{4} = \ln \sqrt{\frac{k(x)}{k_o}} \qquad (3.34)$$

where k_o is a constant. By (3.31), this yields

$$\phi(x) \approx \frac{k(x) - k_o}{k(x) + k_o} \qquad (3.35)$$

and, correspondingly,

$$f(x) \approx \frac{k_o}{k(x)} \quad . \qquad (3.36)$$

Moreover, this result for the phase correction function yields $\hbar k_o$ as the momentum evaluated at the turning point. In addition, this asymptotic form permits $\phi(x)$ to remain within the unit circle and provides $\phi(x)$ with a limiting value of -1 at the classical turning point.

However, all the information of interest to us in determining the particular $\phi(x)$ we seek is in the complex constant k_o and this cannot be directly obtained from the properties of $\phi(x)$ in the asymptotic (semiclassical) domain but requires some means of propagating the exact solution across the intermediate region to the turning point. By showing that the appropriate $f(x)$ has the form (3.36) near the turning point, however, we have definitely excluded the two types of particular solution $f(x)$ to (3.29) which were discussed in Appendix B.

E. Nature of the Fundamental and General Solutions $\phi(x)$ and $f(x)$

Additional insight into the structure of our problem can be obtained if we consider the collection of the various fundamental solutions of the Riccati equations (3.29) and (2.13)(or (2.31)) and the general solutions which can be constructed from these fundamental ones.

For example, if we examine the three asymptotic forms for $f(x)$ in the turning point region (namely the two obtained in Appendix B and the one obtained in the preceding section), we observe that they are distinctly different from each other. The reason for this may

be traced back to the form of the general solution to the Riccati equation$^{(11)}$. Given a function $\psi(x)$ determined by

$$\psi(x) = \frac{g_1(x) + \xi g_2(x)}{g_3(x) + \xi g_4(x)} \tag{3.37}$$

where ξ is a constant, and where $g_1(x)$, $g_2(x)$, $g_3(x)$ and $g_4(x)$ are arbitrary functions, then the constant ξ may be eliminated by obtaining the following Riccati equation for $\psi(x)$:

$$\psi'(x) + Q(x)\psi(x) + R(x)\psi^2(x) = P(x) \tag{3.38}$$

where

$$Q(x) = \{g_1'(x)g_4(x) - g_1(x)g_4'(x) + g_2(x)g_3'(x) - g_2'(x)g_3(x)\}/D(x)$$

$$R(x) = \{g_3(x)g_4'(x) - g_3'(x)g_4(x)\}/D(x) \tag{3.39}$$

$$P(x) = \{g_1'(x)g_2(x) - g_1(x)g_2'(x)\}/D(x)$$

$$D(x) = g_2(x)g_3(x) - g_1(x)g_4(x) \quad .$$

Although four arbitrary functions are employed in defining $\psi(x)$, one of these is superfluous since $\psi(x)$ would remain unchanged if both the numerator and

denominator of (3.37) were to be divided by, for example, $g_3(x)$. Therefore, given four solutions to the differential equation (3.38), namely $\psi_1(x)$, $\psi_2(x)$, $\psi_3(x)$ and $\psi_4(x)$ (corresponding with constants ξ_1, ξ_2, ξ_3 and ξ_4 respectively), it is observed that they are not independent since their "cross ratio"

$$\frac{\{\psi_1(x) - \psi_3(x)\}\{\psi_2(x) - \psi_4(x)\}}{\{\psi_1(x) - \psi_4(x)\}\{\psi_2(x) - \psi_3(x)\}} = \frac{(\xi_1 - \xi_3)(\xi_2 - \xi_4)}{(\xi_1 - \xi_4)(\xi_2 - \xi_3)} \tag{3.40}$$

is a constant. Thus, three solutions to the Riccati equation may be combined to provide a general solution to the equation.

We have found two asymptotic forms for $\phi(x)$ that are valid in the JWKB domain; in addition, we have a technique for obtaining these to arbitrary accuracy. One of these would become very small (going as $k'(x)/4ik^2(x)$) and the other would become very large (going as $4k^2(x)/ik'(x)$). Is there yet a third fundamental solution whose magnitude lies between the moduli of the other two solutions?

Recall that, if $\phi(x)$ satisfies (2.13), then $1/\phi^*(x)$ also satisfies the differential equation. Hence, $\phi(x)$ may possess a solution <u>on</u> the unit circle (since $\phi(x)\phi^*(x)$ would equal unity). Consider, therefore, a solution of the form

$$\phi(x) = -\exp\{-2i\theta(x)\} \tag{3.41}$$

where $\theta(x)$ is a real-valued function which satisfies

$$\theta'(x) = k(x) + \frac{k'(x)}{2k(x)} \operatorname{Sin}\{2\theta(x)\} . \tag{3.42}$$

Then, the wave function has the form

$$y(x) = \exp\{\int_{x_o}^{x} k(x)\operatorname{Cot}[\theta(x)]dx\} . \tag{3.43}$$

Equation (3.42) may be solved asymptotically both far away from and in the vicinity of the turning point. When $k'(x)/2k(x)$ is much smaller than $k(x)$, $\theta(x)$ is given asymptotically by

$$\theta(x) \approx \int_{x_o}^{x} k(x)\, dx . \tag{3.44}$$

Thus, the logarithmic derivative of the wave function becomes

$$\frac{y'(x)}{y(x)} \approx k(x) \operatorname{Cot} \{\int_{x_o}^{x} k(x)\, dx\} . \tag{3.45}$$

The latter may be looked upon as a differential equation and has the immediate solution

$$y(x) \approx \operatorname{Sin} \{\int_{x_o}^{x} k(x)\, dx\} . \tag{3.46}$$

Therefore, this third fundamental solution to the equation for $\phi(x)$ provides the sinusoidal form that characterizes Calogero's solution and the real JWKB approximants. However, in obtaining this relationship, we have sacrificed the conceptual link between quantum mechanics and classical mechanics since it is no longer possible to identify momentum with a continuous function of the spatial variable. For the sake of completeness, consider the turning point region where equation (3.42) becomes

$$\theta'(x) = \frac{k'(x)}{2k(x)} \operatorname{Sin}[2\theta(x)] \quad . \tag{3.47}$$

This equation has the solution

$$\theta(x) = \operatorname{Sin}^{-1} \left\{\frac{2\sqrt{k_o\ k(x)}}{k_o + k(x)}\right\} \tag{3.48}$$

where k_o is a constant, and has the corresponding wave function

$$y(x) \approx \exp\left\{\frac{1}{2} \int_{x_o}^{x} \sqrt{\frac{k(x)}{k_o}}\ [k_o - k(x)]\ dx\right\} \quad . \tag{3.49}$$

It must be emphasized that this is a formal solution only and is not of physical interest. Hence, of the three fundamental solutions for $\phi(x)$, only that which may be obtained by the recursive scheme described earlier may be used to describe the motion of a semiclassical particle.

* * *

The first chapter had presented a number of suggestive arguments for considering solutions to the wave equation in complex exponential form. However, by the end of the second chapter, we had seemingly deviated from this goal and, at the same time, introduced the problem of solving a non-linear equation whose behaviour was more obscure than that of the Schrödinger equation. In this chapter, the solution was cast into the desired exponential form and provided momentum eigenfunctions which would give the classical momentum in the limit $\hbar$ goes to zero. We identified a quantity, namely $f(x)$, as a correction to the phase and amplitude of the wave function. The properties of linear fractional transformations and of the differential equations for $f(x)$ and $\phi(x)$ were used to discuss the relationship between $\phi(x)$ and $f(x)$. This relationship gave rise to a physically desirable initial condition for $\phi(x)$ and provided an upper bound to its magnitude (Appendix A). A convergent iterative scheme for evaluating $\phi(x)$ was provided such that its first-order term was comparable with or superior to the second-order JWKB approximant. In addition, an asymptotic form for $\phi(x)$ valid near the turning point was obtained. Finally, the connection between this solution and that of real-valued wave function approximants was shown. Having discussed the formal properties of this technique, it is now necessary to consider numerical procedures for the rapid numerical calculation of the wave function.

CHAPTER IV

NUMERICAL METHODS

In the preceding chapter, a method for solving a particular type of Riccati equation was proposed: the problem was reformulated as that of solving the infinite set of ancillary equations (3.16). Since discussion of this technique has, to this point, been strictly formal, it will be valuable to qualitatively consider the rationale for its development.

Consider the equation

$$\psi_o(x) = \alpha_o(x) + \beta_o(x)\psi_o^2(x) + \gamma_o(x)\psi_o'(x) \qquad (4.1)$$

where $\alpha_o(x)$, $\beta_o(x)$, and $\gamma_o(x)$ are analytic, small compared with unity, and have slowly varying derivatives for some domain of x. Linearizing this equation and neglecting the derivative term yields $\alpha_o(x)$ as an approximate solution. Thus, the exact solution to this equation may be written as

$$\psi_o(x) = \alpha_o(x) + \psi_1(x) \qquad (4.2)$$

where $\psi_1(x)$ describes the correction to the approximate solution. Inserting this solution into equation (4.1) results in a Ricatti equation of identical form to

(4.1) where the coefficients are given by (3.18). Thus, by linearizing the solution to the original Ricatti equation, we obtain a new Ricatti equation whose solution describes the <u>error</u> in the former. Since the task of solving the latter equation is formally the same as solving the equation for $\psi_o(x)$, this technique may be iterated (where convergent) until convergence is achieved.

This scheme for solving a non-linear equation differs markedly from the JWKB or Langer series. The solution to all orders of this series is linearized; on the other hand, the zeroth order term in the Langer series is the square root of a quantity and, ultimately, manifests itself in the Stokes phenomenon. In addition, to calculate the n-th term in this series, we need only know $\alpha_{n-1}(x)$, $\beta_{n-1}(x)$, and $\gamma_{n-1}(x)$; the JWKB technique requires that all preceding terms be known explicitly. As a consequence, calculations with the linearized iterative scheme are less laborious and, as was noted earlier, more accurate than JWKB approximants of the same order. In the following pages, two techniques for pursuing this technique are described and tested.

A. Rational Function Interpolation

The solution to $\psi_o(x)$ may be written

$$\psi_o(x) = \alpha_o(x) + \alpha_1(x) + \ldots + \alpha_{n-1}(x) + \psi_n(x), \qquad (4.3)$$

where $\alpha_i(x)$, $i=0,1,2,\ldots n-1$ are known and where $\psi_n(x)$ satisfies the Ricatti equation

$$\psi_n(x) = \alpha_n(x) + \beta_n(x)\psi_n^2(x) + \gamma_n(x)\psi_n'(x) \quad . \qquad (4.4)$$

Thus, the problem of solving for $\psi_o(x)$ is reduced to that of solving for $\psi_n(x)$. The subscript n is selected so that the following iterative sequence will converge uniformly in some domain of x:

$$\begin{aligned} \psi_n^{(o)}(x) &= \alpha_o(x) \qquad\qquad (4.5) \\ \psi_n^{(i+1)}(x) &= \alpha_n(x) + \beta_n(x)\psi_n^{(i)}(x)^2 + \gamma_n(x)\psi_n^{(i)'}(x) \qquad i=0,1,2,.. \end{aligned}$$

In the problem of calculating $\phi(x)$, n appears to be unity for maximal numerical stability.

In order to utilize equation (4.5), one must select a finite set of discrete points which are distributed in some regular way in the domain of interest. In order to obtain a numerical estimate of the derivative on a set of discrete points, most numerical

algorithms will use finite difference estimates, that is, truncated Taylor series expressions of low order. In our problem, however, $\phi(x)$ cannot be adequately described by a polynomial of small degree since the general solution to a Riccati equation necessarily has the form of a ratio of two functions. To overcome this difficulty, the set of data points are collocated with a "diagonal rational function of order N," that is

$$R_N(x) = \frac{a_1 + a_2x + \ldots + a_px^{p-1}}{b_1 + b_2x + \ldots + b_qx^{q-1}}$$

$$N = p + q - 1 \qquad (4.6)$$

$$q \leq p \leq q + 1 .$$

Rational functions are widely used$^{(12)}$ in approximation theory and are characterized by an immunity to the rapid fluctuation of derivative that often accompanies ordinary polynomial interpolants. These features make the rational function ideal for this iterative procedure; moreover, it provides a simple algebraic form for $\phi(x)$ instead of the values that $\phi(x)$ assumes on a set of points.

For convenience, the explicit formulation of the iterative procedure for the allowed region is provided

below. For its application to the forbidden region, only the mapping (2.28) need be made.

Recall the equation for the function $\phi(x)$, namely

$$\phi(x) = \frac{g(x)}{h(x)} \{1 - \phi^2(x)\} - \frac{\phi'(x)}{h(x)} \quad , \tag{4.7}$$

where

$$\begin{aligned} h(x) &= 2ik(x) \\ g(x) &= \frac{k'(x)}{2k(x)} \quad . \end{aligned} \tag{4.8}$$

An approximate solution to (4.7), which shall be denoted $\phi^{(o)}(x)$, is given by

$$\phi^{(o)}(x) = \frac{g(x)}{h(x)} \quad . \tag{4.9}$$

Define R(x), which is the residual error in this approximation, by

$$R(x) = \{\frac{g(x)}{h(x)} [1 - \phi^{(o)}(x)^2] - \frac{\phi^{(o)'}(x)}{h(x)} - \phi^{(o)}(x)\} \tag{4.10}$$

and $\mu(x)$, which is the correction to the approximate solution to (4.7),by

$$\mu(x) = \phi(x) - \phi^{(o)}(x) \quad . \tag{4.11}$$

The resulting equation

$$\mu_o(x) \equiv \{1 + 2\,\frac{g(x)}{h(x)}\}^{-1}\; R(x)$$

$$\psi_{i+1}(x) = \{1 + 2\,\frac{g(x)}{h(x)}\}^{-1} \{R(x) - \frac{g(x)}{h(x)}\, \mu_i^2(x) - \frac{\mu_i'(x)}{h(x)}\} \qquad i=0,1,2,.... \tag{4.12}$$

must then be iterated until convergence is obtained.

This procedure may be applied to both bound state and scattering problems; the only significant difference between these is the criterion for selecting the discrete points at which $\phi(x)$ is explicitly evaluated. For bound state problems, these points may be equidistant; this is also the case for part of the scattering domain. However, in the region where the potential "flattens" (i.e. asymptotically tends to zero derivative at infinite separation), the distribution of points should reflect the fact that the more distant portion of the scattering region has much less effect than that nearer the scatterer. To accommodate this behaviour, the density of points should be greatest near the scatterer and least in the region where the potential flattens out. A simple way to assure

this is to require that the distance between successive pairs of points decrease proportionally. For example, one might let

$$\frac{x_{i+2} - x_{i+1}}{x_{i+1} - x_i} = \Gamma \qquad i=0,1,2,\ldots , \tag{4.13}$$

where Γ is a constant which typically lies between two and five. If the endpoints x_o and x_N specified, then x_1 must be selected according to

$$x_1 = x_o + (x_N - x_o) \frac{1 - \Gamma}{1 - \Gamma^{N-1}} \quad . \tag{4.14}$$

The accuracy of this procedure depends upon two factors: the number of data points selected and the number of iterations performed. The number of data points employed provides an upper bound to the accuracy of this technique. The reason for this is that the number of data points corresponds with the number of rational function coefficients and, hence, the number of variable parameters in a truncated Taylor series representation of $\phi(x)$. Typically, ten data points will provide six to eight significant figures in an evaluation of $\phi(x)$. From numerical investigations, the rate of convergence of the iterative scheme depends upon the Euclidean norm of $\phi^{(o)}(x)$ for the domain of x

under consideration. Generally, convergence appears to be assured if the domain of x, namely D, is selected such that

$$||\phi(x)|| < 0.15 \qquad x \varepsilon D \quad . \tag{4.15}$$

For a fixed number of data points, the iteration will converge to the best possible approximation to $\phi(x)$ for the number of variable parameters (that is, data points) used. In order to estimate when convergence, in this case, has been obtained, one need only iterate equations (4.12) until the Euclidean norm of the difference between two successive approximations to $\mu(x)$ is less than some tolerable error. It is important to provide an upper limit to the number of iterations performed in a computer programme; generally, three to ten iterations will provide estimates of $\phi(x)$ to six digits of precision. In comparison with a direct numerical integration of Schrödinger's equation with six-figure accuracy, this technique provides complex wave functions in about one-fourth the time. If $\phi(x)$ is already known, the calculation of the wave function is an order of magnitude faster than a direct numerical integration of the wave equation.

This technique was the first used in order to deduce $\phi(x)$. It adds to the repertory of numerical

analysis a new technique for linearizing and iteratively solving a particular form of the Riccati equation. At the same time, it stimulated the belief that a more simple numerical technique with a greater affinity to analytical methods could be implemented. Finally and of paramount importance, its success confirmed that Schrödinger's equation can indeed be exactly solved with the rapidity of Hamilton's equation, at least in the semiclassical region.

B. Linearized Iterative Sequence

Consider the case of a function U(x) which is analytic, single-valued and non-vanishing in some domain D (the classically allowed or the classially forbidden regions). Then, this function possesses a local Taylor series about every point in D, that is to say U(x), where

$$\begin{aligned} U(x) &= \frac{2m(E - V(x))}{\hbar^2} \\ &= k^2(x) \end{aligned} \tag{4.16}$$

may be associated with a sequence $\{U_i, i=0,1,2,...\}$ where

$$\begin{aligned} U_i &= U(x_1) \qquad \text{if} \quad i=0 \\ &= \frac{d^i}{dx^i} U(x) \Big|_{x=x_1} \qquad \text{if} \quad i=1,2,3,... \quad x_1 \varepsilon D \quad . \end{aligned} \tag{4.17}$$

By making similar associations of derivative sequence with analytic functions a(x), b(x), c(x), the so-called "Leibnitz rule for differentiation" of a product may be written

$$c_i = \sum_{j=0}^{i} \binom{i}{j} a_j b_{i-j} \qquad i=0,1,2,\ldots, \tag{4.18}$$

if c(x) is defined by

$$c(x) = a(x)b(x) \quad . \tag{4.19}$$

Although equations (4.18) and (4.19) are equivalent, in a formal sense, they are very different to computational devices which can manipulate only numerical quantities, but never algebraic functions. The Leibnitz rule can be extended to allow for many other algebraic operations.

If d(x) is the first derivative of c(x), then

$$d_i = c_{i+1} \qquad i=0,1,2,.. \quad . \tag{4.20}$$

If $k^2(x)$ equals U(x), the Leibnitz rule (4.18) may be written

$$\begin{aligned} k_i &= \pm\sqrt{U_o} && \text{if} \quad i=0 \\ &= \frac{U_1}{2k_o} && \text{if} \quad i=1 \\ &= \frac{1}{2k_o}\{U_i - \sum_{j=1}^{i-1} \binom{i}{j} k_j k_{i-j}\} && \text{if } i=2,3,4,\ldots \end{aligned} \tag{4.21}$$

The indeterminacy in the sign is due to the selection of the branch cut. The positive case corresponds with a left going wave, the negative case with a right going wave.

If f(x) is defined to be the reciprocal of g(x), then

$$\begin{aligned} f_i &= 1/g_o \qquad \text{if} \quad i=0 \\ &= -f_o \sum_{j=0}^{i-1} \binom{i}{j} f_j g_{i-j} \qquad \text{if } i=1,2,3,\ldots \; . \end{aligned} \tag{4.22}$$

Extensions of this scheme to the addition of two functions and to the addition or multiplication of a function by a constant are obvious.

Upon examination, it is observed that the linearized iterative scheme described in the previous chapter may be employed to obtain an <u>arbitrary</u> number of terms by using the various forms of Leibnitz rule just described and the recursive features available in modern digital computers. Given a potential where the function value and its first n derivatives are known, $\alpha(x_1)$ and its first n-1 derivatives may be evaluated. In calculating each term in the α series, an additional derivative is lost so that, when $\alpha_{n-1}(x_1)$ is evaluated, none of its derivatives are known. To calculate $\phi(x_1)$ to arbitrary accuracy, it is only necessary to take a

"running sum" of $\alpha_i(x_1)$ function values; no derivative information need be stored. This technique for calculating $\phi(x_1)$ cannot be readily extended to the JWKB or Langer series since, in order to calculate the n-th term, the preceding n-1 terms must be known simultaneously. However, as each term in the α series relies only on the immediately preceding one, this difficulty never arises and it is not necessary to store or manipulate large amounts of numerical data. It must be emphasized, however, that this technique does not provide a simple algebraic form for $\phi(x)$ (unlike the method of rational function interpolants). Instead, it can provide numerical values at discrete points of almost arbitrary accuracy at specified points. If an algebraic form for $\phi(x)$ is desirable, the numerical information provided by this method can be collocated with a rational function or other interpolating function.

This technique has proven to be markedly superior to that of rational function interpolants. It is simpler to use and, for the same domain of x, converges much more rapidly. The explicit three-term form for $\phi(x)$ obtained in equations (3.22) to (3.25) will give $\phi(x)$ correct to seven significant digits in seventy per cent of the allowed region; four or five digits accuracy

is available in eighty-five per cent of this domain. It is vital to note that, as the three-term series is a simple algebraic expression, these results were obtained with only a modest increase in computer time compared with a direct integration of the Hamilton characteristic function. The ten-term series (obtained from the application of the Leibnitz rule to the linearized iterative sequence) would converge to ten-digit accuracy in half of the allowed region; seven-digit accuracy has been obtained for seventy per cent of the region. In the portion of the allowed region where JWKB approximants deteriorated, the α series oscillated and eventually diverged.

In the forbidden region, the success of this technique appeared to be significantly enhanced. Generally speaking, the series would converge when evaluated at the same distance from the turning point as a point in the allowed region but would do so more rapidly. In fact, convergence of ten to sixteen figure accuracy would be typical and would be obtained in less than one-tenth of a second. Moreover, the three-term series was capable of providing the logarithmic derivative of the wave function with ten to twelve digits of precision when evaluated asymptotically far from the turning point. It is essential to note that no known techniques for numerical integration

reliably predict the logarithmic derivative to more than six or eight digits of accuracy. Thus, the linearized iterative technique (or its explicit three-term form) has realized the objective of numerically calculating the wave function with the ease and rapidity one would associate only with the solution to Hamilton's equations.

By the iterative process described in this chapter, we may obtain essentially exact values for the desired function $\phi(x)$ and, hence, for the corresponding exact "pure complex exponential" solution to the Schrödinger equation in the region where a semi-classical (JWKB) approximation would be valid. We have given some brief exemplary data on numerical convergence of the iterative process in the two cases.

Again, we wish to emphasize that the objective of this thesis is not to present a complete set of numerical techniques for calculating the solution $y(x)$ to Schrödinger's equation but to show that, in principle, the exact wave function may be obtained everywhere at a speed controlled by Hamilton's equations and that this is practicable in the region of rapid oscillation in the Schrödinger wave function if we preserve the conceptual link between quantum and classical mechanics in the method employed. This we have done by demonstrating the existence of a smooth

wave mechanical correction function $\phi(x)$ and calculating it "iteratively" in the semiclassical regions. However, for the sake of completeness, we shall briefly discuss the problem of rapid numerical continuation through the turning point region and neighbouring domains where the iterative scheme for $\phi(x)$ fails.

We may begin by recalling that, in the classically forbidden regions, the solution $y(x) = \psi(x)$, say, generated by the $\phi(x)$ iterative scheme is just the regular solution which is normally of interest. In the classically allowed region, the iterative solution $\phi(x)$ to (2.13) and its complex conjugate $\phi^*(x)$ generate a pair of complex exponential solutions $y(x)$, $y^*(x)$, and some (conventionally real) linear combination of these,

$$\psi(x) = ay(x) + a^*y^*(x) \quad , \qquad (4.23)$$

which is the analytic continuation of the solution originated in a forbidden region. To determine the coefficient $\underline{a}$ requires some process for propagating $\psi(x)$ across the region between the two domains where iterative solution of (2.31) or (2.13) can be done.

This region has essentially two distinct parts which must be treated differently: (a) the turning

point region proper, where $|k^2(x)| < |k'(x)|$, and $\phi(x)$ has a form described approximately by (3.35); (b) an intermediate region where $|k^2(x)| \approx |k'(x)|$ and the iterative device converges poorly. In the turning point region proper, a variety of techniques may be considered, including, for example, methods based on various power-series solutions. These will suffice to join a solution $\psi(x)$ coming from the convergence region of the iterative device (2.31) or (2.34) in the non-classical region and carry it across the zero of $k^2(x)$; however, they deteriorate badly as soon as the oscillations of $\psi(x)$ commence in the classically allowed region and, using them, we can at best propagate $\psi(x)$ to its first node. Between this point and the semiclassical domain where the iterative solution for $\phi(x)$ is known lies an "intermediate" region. In this region, several oscillations of $\psi(x)$ may occur so that direct numerical integration of the Schrödinger equation would be too time-consuming. However, in this intermediate region, numerical integration of (2.13) or some smooth related differential equation will become stable as the asymptotic iterative method becomes unsuitable.

CHAPTER V

CONCLUSION

In the preceding chapter, we investigated a set of techniques for isolating a particular solution to the equation for $\phi(x)$, one which asymptotically provided the JWKB approximants. We know that any solution to the equation for $\phi(x)$ furnishes a pair of solutions to the one-dimensional Schrödinger equation and yet there is an especially attractive quality surrounding this particular choice of $\phi(x)$.

In the appendix, we observe that $\phi(x)$ is invariably either inside the unit circle, outside the unit circle, or on the unit circle. In terms of the linear fractional transformation which relates $\phi(x)$ to $f(x)$, the phase correction function is either in the right-half complex plane, in the left-half complex plane, or on the imaginary axis, respectively. Therefore, the theorem and corollaries of Appendix A may be looked upon as a form of conservation principle, that is to say, the preservation of the direction of a quantum mechanical particle's momentum. If, initially, a particle may be described as being predominantly left going ($|\phi(x_o)| < 1$), it is always so. If, initially, a particle may be described as being predominantly

right going ($|\phi(x_o)| > 1$), it is always so. Finally, if a particle may be described as possessing equiprobable left and right going states ($|\phi(x_o)| = 1$), it will always remain so. Of all the left going solutions, the techniques of the preceding chapter provides one which is uniquely that of a <u>pure</u> left going wave, an observation which was verified by comparison with a direct numerical integration of Schrödinger's equation. What then may one conclude about other solutions to $\phi(x)$ which are contained inside the unit circle?

In the third chapter, we saw that a general solution to a Riccati equation could be obtained from three particular solutions. In the case of the equation for $\phi(x)$, one might select, as particular solutions, the one obtained from the linearized iterative sequence, the complex conjugate of its reciprocal, and one which is of unit modulus. It is important to note that the latter solution is characterized by a double wave-frequency clockwise rotation on the unit circle (see equations (3.49) and (3.50)). On the other hand, the solution to $\phi(x)$ which we have sought describes a contour which, commencing with a point on the negative real-axis (corresponding with the zero-force point), proceeds slowly upward, parallel to the

imaginary axis. Then, it follows a sweeping retrograde motion that goes through 180° becoming asymptotically parallel to the imaginary axis as the classical turning point looms nearer. All other solutions to the equation for $\phi(x)$ which are bounded by the unit circle contain a "mixture" of these three fundamental solutions (owing to the linear fractional transformation involved). This has two deleterious effects. It contains some of the character of the unit modulus solution, that is, the double frequency oscillations which have plagued many numerical investigations of the solution to Schrödinger's equation. At the same time, this solution does not provide a pure left going wave but contains a limited amount of right going character. By analogy to classical wave motion, this corresponds to a reflected wave which manifests itself as a form of interference and is typified by a double local wave-frequency. This, then, has the effect of introducing spurious fluctuations in the real and imaginary parts of the logarithmic derivative of the wave function. Thus, the deceptive undulatory appearance of numerical estimates of the quantum mechanical momentum are nothing more than the result of not having selected the correct initial condition for a pure travelling wave. The linearized iterative sequence provides a pure left

or right going wave and, hence, a quantum mechanical momentum which departs from its classical counterpart in a smoothly-varying, non-oscillatory manner. Moreover, it does so in a manner which permits the calculation of the wave function with the ease and rapidity of solving the Hamilton equations of motion.

The strength of this technique is that it embodies a methodological link between the wave and particle descriptions of matter. By reformulating the problem of solving the one-dimensional Schrödinger equation as a correction to an asymptotic form, one preserves the intimate connection between the local and wave mechanical momenta. By confining onself to a particular solution of the resultant Riccati equation, the wave function necessarily becomes the exponential of a modified form of the Hamilton characteristic function. Simultaneously, the wave function becomes,numerically, no more elusive than the solution to the Hamilton-Jacobi equations.

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APPENDIX A

BOUNDING OF $\phi(x)$

Theorem:

If $|\phi(x_o)| < 1$ for some x_o in the classically allowed region D, then $\phi(x)$ is bounded by the unit circle for all x in D.

Proof:

The function $\phi(x)$ is defined by

$$\phi(x) = \frac{k'(x)}{4ik^2(x)}\{1-\phi^2(x)\} - \frac{\phi'(x)}{2ik(x)} \quad . \tag{A.1}$$

To $\phi(x)$ associate a real-valued non-negative modulus $r(x)$ and a real-valued phase $\theta(x)$ such that

$$\phi(x) = r(x)\exp\{i\theta(x)\} \quad . \tag{A.2}$$

Coupled equations in $r(x)$ and $\theta(x)$ arise, namely

$$\begin{aligned} r'(x) &= \frac{k'(x)}{2k(x)}\{1 - r^2(x)\}\,\mathrm{Cos}\{\theta(x)\} \\ \theta'(x) &= -2k(x) - \frac{k'(x)}{2k(x)}\,\mathrm{Sin}[\theta(x)]\,\frac{1+r^2(x)}{r(x)} \quad . \end{aligned} \tag{A.3}$$

Given the initial condition

$$r_o = r(x_o) < 1 \tag{A.4}$$

a general solution to the first equation in (A.3) is

$$r(x) = \frac{\exp u(x) - c}{\exp u(x) + c} \tag{A.5}$$

where u(x) is given by

$$u(x) = 2 \int_{x_o}^{x} \frac{k'(x)}{2k(x)} \operatorname{Cos}\{\theta(x)\}\, dx \tag{A.6}$$

and where c is a real-valued constant; the initial condition confines c to the value

$$c = \frac{1 - r_o}{1 + r_o} \quad . \tag{A.7}$$

Since $r_o < 1$, c must be positive. For an arbitrary value of $x \varepsilon D$, (A.5) may be rewritten as

$$1 - r(x) = c\{1 + r(x)\} \exp\{-u(x)\} \quad . \tag{A.8}$$

But, the right-hand side of the latter is positive definite and

$$1 - r(x) > 0 \tag{A.9}$$

completing the proof.

* * *

Corollary:

If $|\phi(x_o)| > 1$ for some $x_o \varepsilon D$, then $|\phi(x)| > 1$ for all $x \varepsilon D$.

Proof:

Define a function $\hat{\phi}(x)$ by

$$\hat{\phi}(x) = 1/\phi^*(x) \quad . \tag{A.10}$$

By direct substitution, it is observed that $\hat{\phi}(x)$ satisfies (A.1) and that $|\hat{\phi}(x_o)| < 1$. By the preceding theorem, $|\hat{\phi}(x)| < 1$ for all $x \varepsilon D$. Thus, $|\phi(x)| > 1$ for all $x \varepsilon D$.

* * *

Corollary:

If $|\phi(x_o)| = 1$ for some $x_o \varepsilon D$, then $|\phi(x)| = 1$ for all $x \varepsilon D$.

Proof:

Write $\phi(x)$ in polar form (A.2); then, $r(x)$ is given by (A.5) where, by (A.7), c is identically zero. Therefore, from (A.5),

$$r(x) = 1 \tag{A.11}$$

for all $x \varepsilon D$.

APPENDIX B

TWO ASYMPTOTIC FORMS FOR f(x)

In calculating f(x) at the turning point, one would prefer to employ the iterative scheme on the differential equation for the phase correction function. Unfortunately, the derivative of $\alpha(x)$ for this case is not slowly varying. So, for the solution to

$$f(x) = \frac{ik^2(x)}{k'(x)} \{1 - f^2(x)\} - \frac{k(x)}{k'(x)} f'(x) \quad , \qquad (B.1)$$

it is not sufficient to say that an asymptotic solution to f(x) valid in a neighbourhood about the turning point is $ik^2(x)/k'(x)$, since the derivative of this quantity is not slowly varying. A more flexible asymptotic form is $cik^2(x)/k'(x)$ where c is a constant that is to be determined. Detailed calculations show c to be 1/4 and that

$$f(x) \approx \frac{ik^2(x)}{4k'(x)} \quad . \qquad (B.2)$$

The corresponding wave function is

$$y(x) = \exp \{- \frac{1}{2} \int^x \frac{k^4(x')\ dx'}{\frac{d}{dx'}[k^2(x')]}\} \qquad (B.3)$$

and, in the case of a linear turning point,

$$k^2(x) = x \tag{B.4}$$

this becomes

$$y(x) \approx \exp[-x^3/6] \quad . \tag{B.5}$$

This solution is related to the Airy functions by

$$y(x) = \{A_i(-x) + \frac{B_i(-x)}{\sqrt{3}}\} \frac{\Gamma(\frac{1}{3})\; 3^{1/3}}{2} \quad . \tag{B.6}$$

Recall that, in the case of the differential equation for $\phi(x)$, the function $1/\phi^*(x)$ is also a solution. This suggests that some constant times $k'(x)/ik^2(x)$ might be an asymptotic solution for $f(x)$. Similar calculations show that $f(x)$ may be given approximately by

$$f(x) \approx -\frac{2ik'(x)}{k^2(x)} \tag{B.7}$$

and that the wave function becomes

$$y(x) = \exp\{\int^x \frac{\frac{d}{dx'}[k^2(x')]}{k^2(x')} dx'\} \quad . \tag{B.8}$$

In the case of a linear turning point, the latter becomes

$$y(x) \approx x \quad , \tag{B.9}$$

which is related to the Airy functions by

$$y(x) \approx \{A_i(-x) - \frac{B_i(-x)}{\sqrt{3}}\} \frac{\Gamma(\frac{1}{3})\ 3^{1/3}}{2} \quad . \qquad \text{(B.10)}$$

Unfortunately, these asymptotic forms do not conform to the type of solution one would require if it were to be, at the same time, a momentum operator eigenfunction. The momentum of a semi-classical particle "tunneling" through the turning point into the forbidden region should have a finite but non-vanishing "momentum." Therefore, the solutions obtained here for f(x) must be discarded in favour of one which behaves like some constant terms 1/k(x) in the vicinity of the turning point.

APPENDIX C

SOME ILLUSTRATIVE NUMERICAL RESULTS

Having made a number of comments regarding the properties of the linearized iterative sequence, we give here some illustrative examples of numerical results which demonstrate the ease and accuracy inherent to this technique. As a model, the twenty-fourth level of a simple harmonic oscillator potential is tested below. There is, however, no reason to suspect that these results are peculiar to the harmonic oscillator; in fact, this problem is a "worst possible case" since $[k'(x)/k^2(x)]$ does not go to zero as strongly for this potential as for most physically realistic potentials.

* * *

Classically Forbidden Region

In the case of the forbidden region, we numerically integrate the Schrödinger equation with a fourth order Runge Kutta from 15.0 to the turning point (7.0). At selected points (denoted X), we output the logarithmic derivative (YPRIME/Y) from the exact numerical integration (EXACT), from a second order JWKB calculation (WKB) and from a three-term α series for ϕ

(SERIES). Similarly, the exact and series estimates of f(x) (denoted F) and $\phi(x)$ (denoted PHI) are given. For example, at 14.9 (which is "far" from the turning point), we have

```
X                     1.489999999999999D 01
YPRIME/Y(EXACT)      -1.319616513368636D 01
YPRIME/Y(WKB)        -1.319638767016770D 01
YPRIME/Y(SERIES)     -1.319614880306987D 01
F(EXACT)              1.003256861145154D 00
F(SERIES)             1.003255619587257D 00
-------------------------------------------
PHI(EXACT)           -1.625783097676806D-03
PHI(SERIES)          -1.625164335207708D-03
```

Consider, also, the following estimate for $\phi(x)$ in terms of a nine-term α series. Note the extraordinary rate of convergence of the series.

```
PHI                  -1.6251603687D-03
SERIES
----------------------------------------------
      -1.6368898958D-03
       1.1904704912D-05
      -1.7916186870D-07
       4.1058276338D-09
      -1.2643232256D-10
---------------------------------------------
       4.8882228455D-12
      -2.2741405616D-13
       1.2365581691D-14
      -7.6938699336D-16
```

By direct comparison, it may be noted that the three-term α series estimate of $\phi(x)$ is more accurate than the exact numerical integration! Indeed, far from the turning point, the three-term series will typically provide ten digit accuracy.

Now, let us look at some results obtained significantly closer to the turning point but still in the asymptotic domain, namely

```
X                       1.099999999999999D 01
YPRIME/Y(EXACT)        -8.560416092333452D 00
YPRIME/Y(WKB)          -8.561670263127453D 00
YPRIME/Y(SERIES)       -8.560420804163676D 00
F(EXACT)                1.008854711444572D 00
F(SERIES)               1.008855266739089D 00
---------------------------------------------
PHI(EXACT)             -4.407840643788936D-03
PHI(SERIES)            -4.408115848716355D-03
```

and

```
PHI                   -4.4078401422D-03

SERIES
-----------------------------------------
      -4.5012584451D-03

       9.7542560002D-05

      -4.4011171042D-06

       3.0178963824D-07

      -2.7741564162D-08
-----------------------------------------
       3.1961226163D-09

      -4.4252879354D-10

       7.1548228631D-11

      -1.3228271295D-11
-----------------------------------------
```

At this point, the rate of convergence of the α series is no longer so rapid and the estimate of ϕ obtained from the three-term α series is less precise than that obtained from the numerical integration. However, it should be noted that the three-term α series evaluation of $\phi(x)$ is correct to the seventh significant figure and, thus, is sufficiently accurate for most physical applications.

Consider, finally, the application of this technique to a point in the near vicinity of the turning point. Here, the α series is asymptotic and begins to diverge after the sixth term, namely

```
X                      7.999999999999993D 00

YPRIME/Y(EXACT)       -4.108657178764820D 00

YPRIME/Y(WKB)         -4.139650012874071D 00

YPRIME/Y(SERIES)      -4.115851259271729D 00

F(EXACT)               1.060850721908783D 00

F(SERIES)              1.062708225508418D 00
----------------------------------------------
PHI(EXACT)            -2.952699157774166D-02

PHI(SERIES)           -3.040091891472582D-02
```

and

```
PHI                     -3.1253411577D-02

SERIES
-------------------------------------------
      -3.4426518633D-02

       6.5807585204D-03

      -2.5600978225D-03

       1.4974732945D-03

      -1.1671202290D-03
-------------------------------------------
       1.1356912060D-03

      -1.3242384447D-03

       1.7987116419D-03

      -2.7880711108D-03
-------------------------------------------
```

It was observed that, for the case of the twenty-fourth harmonic oscillator level, the three-term α series was sufficiently accurate in estimating $\phi(x)$ for x greater

than 9.0 to satisfy any reasonable computational requirements in calculating the wave function in the forbidden region, at the same time, provided the solution with the speed of solving Hamilton's equations.

* * *

Classically Allowed Region

The α series is rapidly convergent for seventy per cent of the allowed domain. Fifteen-term α series are given below for a set of points. (Note that the numerical values for ϕ and α_i have two components corresponding with real and imaginary parts.)

```
X            0.0
PHI         -5.200761498933640D-05    0.0
SERIES
------------------------------------------
     1:      0.0                      0.0
     2:     -5.206164098292376D-05    0.0
------------------------------------------
     3:      0.0                      0.0
     4:      5.420899477982009D-08    0.0
     5:      8.457701747013455D-13    0.0
------------------------------------------
     6:     -1.851437712452998D-10    0.0
     7:     -8.798747020599331D-15    0.0
     8:      1.321319924872674D-12    0.0
     9:      1.271007610222153D-16    0.0
    10:     -1.612967304265969D-14    0.0
    11:     -2.609962914660366D-18    0.0
------------------------------------------
    12:      3.004587879310238D-16    0.0
    13:      7.345087590179455D-20    0.0
    14:     -7.931679272439819D-18    0.0
    15:     -2.729655603171690D-21    0.0
```

```
X          5.000000000000000D-01
PHI       -5.334754054386651D-05   3.668499185824523D-04

SERIES

     1:    0.0                     3.672383969432988D-04
     2:   -5.340617432018050D-05   4.952726728337742D-11

     3:   -2.159243554017243D-11  -3.898839904407712D-07
     4:    5.887170249998136D-08  -6.435407334456809D-12
     5:    1.074109300616147D-12   1.372545342450028D-09

     6:   -2.191191765801522D-10   6.916380820031524D-14
     7:   -1.218020878803673D-14  -1.020431804211840D-11
     8:    1.747111218149385D-12  -1.048489826877622D-15
     9:    1.987252990734549D-16   1.310974355079159D-13
    10:   -2.431688981864322D-14   2.284542309319157D-17
    11:   -4.700912399284346D-18  -2.595174131523729D-15

    12:    5.247607738295109D-16  -6.887961844012334D-19
    13:    1.544944850433668D-19   7.347413453867652D-17
    14:   -1.624403578082846D-17   2.766456516611670D-20
    15:   -6.770777592382257D-21  -2.822966126251339D-18


X          3.499999999999999D 00
PHI       -1.839591574706930D-04   3.916131412822352D-03
SERIES

     1:    0.0                     3.927552851630106D-03
     2:   -1.851137678364827D-04   6.058700889518091D-08
     3:   -8.550124066850893D-09  -1.163373757162548D-05
     4:    1.188146895003066D-06  -1.340168754848880D-09
     5:    2.436751523321574D-10   1.579724269196933D-07

     6:   -2.635821876978867D-08   5.148062574812074D-11
     7:   -1.246510728695226D-11  -5.267044640470659D-09
     8:    1.227738657769924D-09  -3.411541075230715D-12
     9:    1.042695162795445D-12   3.269486121581825D-10
    10:   -9.793345831121491D-11   3.522410085159013D-13
    11:   -1.303803337814171D-13  -3.258991388551702D-11

    12:    1.192867340680830D-11  -5.248681768396654D-14
    13:    2.283439955431047D-14   4.762844270115890D-12
    14:   -2.060104268565904D-12   1.067673361852257D-14
    15:   -5.339623152031789D-15  -9.596001646399439D-13
```

It has been observed, heuristically, that the allowed region may be considered to have three distinct regions. First, there is the region where the α series effectively converges. This is approximately seventy per cent of the allowed region and the three-term series for $\phi(x)$ will give seven-figure wave functions in most of this domain. Then, there is a region (about twenty per cent of the allowed domain) where the α series is asymptotic. Finally, the remaining ten per cent of the domain (namely that localized about the turning points) is completely divergent. However, it must be emphasized that it is in the region where the linearized iterative sequence is successful that numerical integration techniques are most impaired and that it is here that we can readily solve the one-dimensional Schrödinger equation with the speed of Hamilton's equation. Moreover, we have already established stable numerical integration techniques which allow us to extend the solution to the turning point.